CHBE 305

COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING

Spring 2017

Instructor

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Office Hours: MW 4 - 5 PM

Course Contents

1. **Introduction**: Approximations and round-off errors; truncation errors; Taylor series.
2. **Systems of linear algebraic equations**: Introduction; Gauss elimination, LU decomposition; inversion of matrices; error analysis and system condition; band matrices; iterative solution; Gauss-Seidel method.
3. **Curve fitting**: Least squares regression; linear regression; polynomial regression; multiple linear regression; general linear least squares; nonlinear regression. Interpolation; spline interpolation.
4. **Non-linear equations**: Bisection method; false-position method; simple fixed-point iteration; Newton-Raphson method; secant method; multiple roots; systems on nonlinear equations; roots of polynomials.
5. **Numerical integration**: Trapezoidal and Simpson's rules; Romberg integration; Gauss quadrature.
6. **Ordinary differential equations**: Euler's methods; Runge-Kutta methods; adaptive Runge-Kutta methods; systems of equations; stiffness; multistep methods; general methods for boundary values problems; eigenvalue problems.

Textbook

S. C. Chapra and R.R. Canale, "Numerical methods for Engineers." 7th Edition, McGraw-Hill (2015).

Recitation Sessions (Computer Labs)

A 2-hour recitation session will be held every week. The class will be divided in sections for the recitations. Attendance of recitations is mandatory.

Homework Assignments

Six to eight homework problem sets will be assigned during the semester. Problems will involve both theoretical analysis and computer programing. Students should use MATLAB for the solution of homework problems.

Homework Policy

- Late homework will be penalized, unless prior permission has been obtained from the instructor.
- Homework that is more than four days late will not be accepted.
- You can get up to two "free extensions" of homework due dates by notifying the instructor and the TAs in advance of the due date. For each of the free extensions, you may push the due date by no more than two class periods. You cannot use both free extensions for the same homework.
- There will be no "regrades."
- The submission and grading procedures are described in detail in a separate document posted on OwlSpace.

Quizzes

There will be three short quizzes after the completion of major topics to test the students' understanding of key concepts. The quizzes will not require the use of computers and their dates are listed on the course schedule.

Tests

There will be two comprehensive tests on February 27 and April 21 (last day of classes). Again, the tests will not require the use of computers.

Team Project

Students will work in teams to design a chemical reactor system that meets certain specifications. Each team will:

- prepare a 2-page preliminary written report (due on February 24, 2017),
- make a formal presentation of their design (tentatively scheduled for April 24-25, 2017), and
- submit a final written report by the last day of finals (May 3, 2017).

During the week of February 27, students will work with CWOVC coaches who will review their 2-page written report on the project and provide feedback (not grades) to help the teams improve their writing. A revised version of this assignment will be due on

March 10 and this is the version that will be graded. Finally, during the last two week of classes, the teams will work with CWOVC coaches to prepare their final project presentations.

Professional Communications

The professional communication component of this course will include two lectures presented by team members from Rice's Center for Oral, Written and Visual Communication (CWOVC):

- A lecture on creating effective graphics (January 27)
- A lecture on designing effective presentations (March 20)

Grading Policy

- Homework: 30%
- Quizzes: 10% (5% for each of the best 2 out of 3)
- Project: 30%
- Tests: 30% (15% for each test

Note that the weights of the course components may change. The raw scores earned on each of the assignments (homework, quizzes, project and tests) will be converted to standard T-scores. The final course grade will then be computed by averaging all the T-scores according to the above weights.

Honor Code Policy

“Students may talk to each other, the course assistant(s), and the instructor about any assignment in the course that is not specifically designated as pledged. This assistance is limited to a discussion about the mathematical concepts involved in solving the problem. Students are not allowed to share computer codes and calculation details, or to consult another student's solution (even from a previous CHBE 305 or other numerical methods class). Submitted solutions to assignments may not be copied from any source.”

ADA Statement

Any student with a documented disability needing academic adjustments or accommodations is requested to speak with the instructor during the first two weeks of class. All discussions will remain confidential. Students with disabilities will need to also contact Disability Support Services in the Ley Student Center.